

# INTERNATIONAL SEARCH REPORT

Inte I Application No  
PCT/US2004/020992

## A. CLASSIFICATION OF SUBJECT MATTER

IPC 7 G06F19/00

According to International Patent Classification (IPC) or to both national classification and IPC

## B. FIELDS SEARCHED

Minimum documentation searched (classification system followed by classification symbols)  
IPC 7 G06F

Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched

Electronic data base consulted during the international search (name of data base and, where practical, search terms used)

EPO-Internal, WPI Data, PAJ, INSPEC, IBM-TDB

## C. DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	BRIEM H ET AL: "Molecular similarity based on DOCK-generated fingerprints" JOURNAL OF MEDICINAL CHEMISTRY, AMERICAN CHEMICAL SOCIETY, WASHINGTON, US, vol. 17, no. 39, 1996, pages 3401-3408, XP002078005 ISSN: 0022-2623 page 3401, left-hand column, paragraph 1 - page 3403, left-hand column, paragraph 3 page 3406, right-hand column, paragraph 3 - page 3408, left-hand column, paragraph 1 abstract	1-76
X	US 2002/072887 A1 (SZALMA SANDOR ET AL) 13 June 2002 (2002-06-13) paragraphs '0006! - '0017! paragraphs '0028! - '0038! abstract; claims 1-11,16; figures 3-5 ----- -/-	1-76

☒ Further documents are listed in the continuation of box C.

☒ Patent family members are listed in annex.

### \* Special categories of cited documents :

- \*A\* document defining the general state of the art which is not considered to be of particular relevance
- \*E\* earlier document but published on or after the international filing date
- \*L\* document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another citation or other special reason (as specified)
- \*O\* document referring to an oral disclosure, use, exhibition or other means
- \*P\* document published prior to the international filing date but later than the priority date claimed

- \*T\* later document published after the international filing date or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention
- \*X\* document of particular relevance; the claimed invention cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone
- \*Y\* document of particular relevance; the claimed invention cannot be considered to involve an inventive step when the document is combined with one or more other such documents, such combination being obvious to a person skilled in the art.
- \*&\* document member of the same patent family

Date of the actual completion of the international search

30 August 2005

Date of mailing of the international search report

07/09/2005

Name and mailing address of the ISA

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## C.(Continuation) DOCUMENTS CONSIDERED TO BE RELEVANT

Category *	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	BAJORATH J: "Selected concepts and investigations in compound classification, molecular descriptor analysis, and virtual screening." JOURNAL OF CHEMICAL INFORMATION AND COMPUTER SCIENCES. 2001 MAR-APR, vol. 41, no. 2, March 2001 (2001-03), pages 233-245, XP002342110 ISSN: 0095-2338 page 233, right-hand column, paragraph 2 page 237, left-hand column, last paragraph - right-hand column, paragraph 3 page 238, right-hand column, paragraph 2 -----	1-76
P,X	DENG ZHAN ET AL: "Structural interaction fingerprint (SIFt): a novel method for analyzing three-dimensional protein-ligand binding interactions." JOURNAL OF MEDICINAL CHEMISTRY. 15 JAN 2004, vol. 47, no. 2, 15 January 2004 (2004-01-15), pages 337-344, XP002342111 ISSN: 0022-2623 the whole document -----	1-76

# INTERNATIONAL SEARCH REPORT

Information on patent family members

International Application No

PCT/US2004/020992

Patent document  
cited in search report

Publication  
date

Patent family  
member(s)

Publication  
date

US 2002072887 A1 13-06-2002 NONE

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